

Under the Paperwork Reduction Act of 1995, no persons are required to respond to a collection of information unless it contains a valid OMB control number.

<b>Application Data Sheet 37 CFR 1.76</b>		<b>Attorney Docket Number</b>	7875-015
		<b>Application Number</b>	
<b>Title of Invention</b>	METHOD FOR ENERGY RANKING OF MOLECULAR CRYSTALS USING DFT CALCULATIONS AND EMPIRICAL VAN DER WAALS POTENTIALS		
<p>The application data sheet is part of the provisional or nonprovisional application for which it is being submitted. The following form contains the bibliographic data arranged in a format specified by the United States Patent and Trademark Office as outlined in 37 CFR 1.76.</p> <p>This document may be completed electronically and submitted to the Office in electronic format using the Electronic Filing System (EFS) or the document may be printed and included in a paper filed application.</p>			

**Secrecy Order 37 CFR 5.2**

<input type="checkbox"/>	Portions or all of the application associated with this Application Data Sheet may fall under a Secrecy Order pursuant to 37 CFR 5.2 (Paper filers only. Applications that fall under Secrecy Order may not be filed electronically.)
--------------------------	---

**Applicant Information:**

<b>Applicant 1</b>					<input type="button" value="Remove"/>
<b>Applicant Authority</b>		<input checked="" type="radio"/> Inventor		<input type="radio"/> Legal Representative under 35 U.S.C. 117	<input type="radio"/> Party of Interest under 35 U.S.C. 118
<b>Prefix</b>	<b>Given Name</b>	<b>Middle Name</b>	<b>Family Name</b>	<b>Suffix</b>	
	Marcus	A.	Neumann		
<b>Residence Information (Select One)</b> <input type="radio"/> US Residency <input checked="" type="radio"/> Non US Residency <input type="radio"/> Active US Military Service					
<b>City</b>	St-Germain-en-Laye	<b>Country Of Residence</b>	FR		
<b>Citizenship under 37 CFR 1.41(b) <sup>1</sup></b>	DE				
<b>Mailing Address of Applicant:</b>					
<b>Address 1</b>	30bis, rue du Vieil Abreuvoir				
<b>Address 2</b>					
<b>City</b>	St-Germain-en-Laye	<b>State/Province</b>			
<b>Postal Code</b>	F-78100	<b>Country</b>	FR		
All Inventors Must Be Listed - Additional Inventor Information blocks may be generated within this form by selecting the Add button.					
					<input type="button" value="Add"/>

**Correspondence Information:**

Enter either Customer Number or complete the Correspondence Information section below. For further information see 37 CFR 1.33(a).			
<input type="checkbox"/> An Address is being provided for the correspondence Information of this application.			
<b>Customer Number</b>	20575		
<b>Email Address</b>	docketing@techlaw.com	<input type="button" value="Add Email"/>	<input type="button" value="Remove Email"/>

**Application Information:**

<b>Title of the Invention</b>	METHOD FOR ENERGY RANKING OF MOLECULAR CRYSTALS USING DFT CALCULATIONS AND EMPIRICAL VAN DER WAALS POTENTIALS		
<b>Attorney Docket Number</b>	7875-015	<b>Small Entity Status Claimed</b>	<input checked="" type="checkbox"/>
<b>Application Type</b>	Nonprovisional		
<b>Subject Matter</b>	Utility		
<b>Suggested Class (if any)</b>		<b>Sub Class (if any)</b>	
<b>Suggested Technology Center (if any)</b>			
<b>Total Number of Drawing Sheets (if any)</b>	10	<b>Suggested Figure for Publication (if any)</b>	

Under the Paperwork Reduction Act of 1995, no persons are required to respond to a collection of information unless it contains a valid OMB control number.

<b>Application Data Sheet 37 CFR 1.76</b>		Attorney Docket Number	7875-015
		Application Number	
Title of Invention	METHOD FOR ENERGY RANKING OF MOLECULAR CRYSTALS USING DFT CALCULATIONS AND EMPIRICAL VAN DER WAALS POTENTIALS		

**Publication Information:**
☐ Request Early Publication (Fee required at time of Request 37 CFR 1.219)

☐ Request Not to Publish. I hereby request that the attached application not be published under 35 U.S.C. 122(b) and certify that the invention disclosed in the attached application has not been and will not be the subject of an application filed in another country, or under a multilateral agreement, that requires publication at eighteen months after filing.

**Representative Information:**

Representative information should be provided for all practitioners having a power of attorney in the application. Providing this information in the Application Data Sheet does not constitute a power of attorney in the application (see 37 CFR 1.32). Enter either Customer Number or complete the Representative Name section below. If both sections are completed the Customer Number will be used for the Representative Information during processing.

Please Select One: ☒ Customer Number ☐ US Patent Practitioner ☐ US Representative (37 CFR 11.9)

Customer Number 20575

**Domestic Priority Information:**

This section allows for the applicant to claim benefit under 35 U.S.C. 119(e), 120, 121, or 365(c). Providing this information in the application data sheet constitutes the specific reference required by 35 U.S.C. 119(e) or 120, and 37 CFR 1.78(a)(2) or CFR 1.78(a)(4), and need not otherwise be made part of the specification.

Prior Application Status

[Remove](#)

Application Number

Continuity Type

Prior Application Number

Filing Date (YYYY-MM-DD)

Additional Domestic Priority Data may be generated within this form by selecting the Add button.

[Add](#)

**Foreign Priority Information:**

This section allows for the applicant to claim benefit of foreign priority and to identify any prior foreign application for which priority is not claimed. Providing this information in the application data sheet constitutes the claim for priority as required by 35 U.S.C. 119(b) and 37 CFR 1.55(a).

[Remove](#)

Application Number

Country <sup>1</sup>

Parent Filing Date (YYYY-MM-DD)

Priority Claimed

PCTEP2005050778

WO

2005-02-24

☒ Yes ☐ No

[Remove](#)

Application Number

Country <sup>1</sup>

Parent Filing Date (YYYY-MM-DD)

Priority Claimed

04290701.4

EP

2004-03-15

☒ Yes ☐ No

Additional Foreign Priority Data may be generated within this form by selecting the Add button.

[Add](#)

Under the Paperwork Reduction Act of 1995, no persons are required to respond to a collection of information unless it contains a valid OMB control number.

<b>Application Data Sheet 37 CFR 1.76</b>		<b>Attorney Docket Number</b>	7875-015
		<b>Application Number</b>	
<b>Title of Invention</b>	METHOD FOR ENERGY RANKING OF MOLECULAR CRYSTALS USING DFT CALCULATIONS AND EMPIRICAL VAN DER WAALS POTENTIALS		

**Assignee Information:**

Providing this information in the application data sheet does not substitute for compliance with any requirement of part 3 of Title 37 of the CFR to have an assignment recorded in the Office.

**Assignee 1**

Remove

If the Assignee is an Organization check here. ☒

**Organization Name** AVANT-GARDE MATERIALS SIMULATION SARL

**Mailing Address Information:**

**Address 1** 30bis, rue du Vieil Abreuvor

**Address 2**

**City** St-Germain-en-Laye

**State/Province**

**Country** FR

**Postal Code**

F-78100

**Phone Number** 5032223613

**Fax Number**

5032744622

**Email Address** docketing@techlaw.com

Additional Assignee Data may be generated within this form by selecting the Add button.

Add

**Signature:**

A signature of the applicant or representative is required in accordance with 37 CFR 1.33 and 10.18. Please see 37 CFR 1.4(d) for the form of the signature.

<b>Signature</b>	/Stephen S. Ford/		<b>Date (YYYY-MM-DD)</b>	2006-09-14	
<b>First Name</b>	Stephen	<b>Last Name</b>	Ford	<b>Registration Number</b>	35139

This collection of information is required by 37 CFR 1.76. The information is required to obtain or retain a benefit by the public which is to file (and by the USPTO to process) an application. Confidentiality is governed by 35 U.S.C. 122 and 37 CFR 1.14. This collection is estimated to take 23 minutes to complete, including gathering, preparing, and submitting the completed application data sheet form to the USPTO. Time will vary depending upon the individual case. Any comments on the amount of time you require to complete this form and/or suggestions for reducing this burden, should be sent to the Chief Information Officer, U.S. Patent and Trademark Office, U.S. Department of Commerce, P.O. Box 1450, Alexandria, VA 22313-1450. DO NOT SEND FEES OR COMPLETED FORMS TO THIS ADDRESS. **SEND TO: Commissioner for Patents, P.O. Box 1450, Alexandria, VA 22313-1450.**

## Privacy Act Statement

The Privacy Act of 1974 (P.L. 93-579) requires that you be given certain information in connection with your submission of the attached form related to a patent application or patent. Accordingly, pursuant to the requirements of the Act, please be advised that: (1) the general authority for the collection of this information is 35 U.S.C. 2(b)(2); (2) furnishing of the information solicited is voluntary; and (3) the principal purpose for which the information is used by the U.S. Patent and Trademark Office is to process and/or examine your submission related to a patent application or patent. If you do not furnish the requested information, the U.S. Patent and Trademark Office may not be able to process and/or examine your submission, which may result in termination of proceedings or abandonment of the application or expiration of the patent.

The information provided by you in this form will be subject to the following routine uses:

1. The information on this form will be treated confidentially to the extent allowed under the Freedom of Information Act (5 U.S.C. 552) and the Privacy Act (5 U.S.C. 552a). Records from this system of records may be disclosed to the Department of Justice to determine whether the Freedom of Information Act requires disclosure of these records.
2. A record from this system of records may be disclosed, as a routine use, in the course of presenting evidence to a court, magistrate, or administrative tribunal, including disclosures to opposing counsel in the course of settlement negotiations.
3. A record in this system of records may be disclosed, as a routine use, to a Member of Congress submitting a request involving an individual, to whom the record pertains, when the individual has requested assistance from the Member with respect to the subject matter of the record.
4. A record in this system of records may be disclosed, as a routine use, to a contractor of the Agency having need for the information in order to perform a contract. Recipients of information shall be required to comply with the requirements of the Privacy Act of 1974, as amended, pursuant to 5 U.S.C. 552a(m).
5. A record related to an International Application filed under the Patent Cooperation Treaty in this system of records may be disclosed, as a routine use, to the International Bureau of the World Intellectual Property Organization, pursuant to the Patent Cooperation Treaty.
6. A record in this system of records may be disclosed, as a routine use, to another federal agency for purposes of National Security review (35 U.S.C. 181) and for review pursuant to the Atomic Energy Act (42 U.S.C. 218(c)).
7. A record from this system of records may be disclosed, as a routine use, to the Administrator, General Services, or his/her designee, during an inspection of records conducted by GSA as part of that agency's responsibility to recommend improvements in records management practices and programs, under authority of 44 U.S.C. 2904 and 2906. Such disclosure shall be made in accordance with the GSA regulations governing inspection of records for this purpose, and any other relevant (i.e., GSA or Commerce) directive. Such disclosure shall not be used to make determinations about individuals.
8. A record from this system of records may be disclosed, as a routine use, to the public after either publication of the application pursuant to 35 U.S.C. 122(b) or issuance of a patent pursuant to 35 U.S.C. 151. Further, a record may be disclosed, subject to the limitations of 37 CFR 1.14, as a routine use, to the public if the record was filed in an application which became abandoned or in which the proceedings were terminated and which application is referenced by either a published application, an application open to public inspections or an issued patent.
9. A record from this system of records may be disclosed, as a routine use, to a Federal, State, or local law enforcement agency, if the USPTO becomes aware of a violation or potential violation of law or regulation.